



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 23, 2022 – 06:44 PM JST

PDB ID : 7EXR
Title : Crystal structure of alkaline alpha-galactosidase D383A mutant from *Arabidopsis thaliana* complexed with Stachyose.
Authors : Chuankhayan, P.; Guan, H.H.; Lin, C.C.; Chen, N.C.; Huang, Y.C.; Yoshimura, M.; Nakagawa, A.; Lee, R.H.; Chen, C.J.
Deposited on : 2021-05-28
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

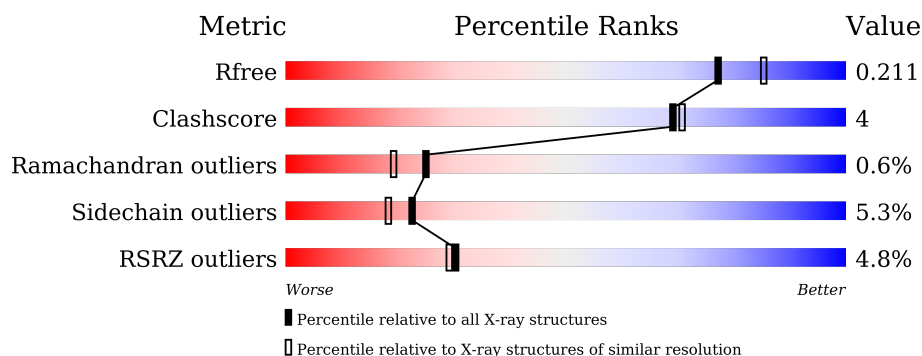
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	749	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	749	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>..</div> </div> </div>
2	C	4	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>
2	D	4	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TTV	C	1	X	-	-	X
2	ZCD	C	3	X	-	-	-
2	TTV	D	1	X	-	-	-
2	ZCD	D	3	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11874 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

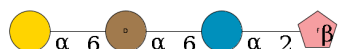
- Molecule 1 is a protein called Probable galactinol–sucrose galactosyltransferase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	718	Total	C	N	O	S	0	0	0
			5620	3573	969	1049	29			
1	A	718	Total	C	N	O	S	0	0	0
			5620	3573	969	1049	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	302	ARG	LYS	conflict	UNP Q8RX87
B	383	ALA	ASP	engineered mutation	UNP Q8RX87
A	302	ARG	LYS	conflict	UNP Q8RX87
A	383	ALA	ASP	engineered mutation	UNP Q8RX87

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-alpha-D-idopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-psicofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			
2	D	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	328	Total	O	0	0
			328	328		

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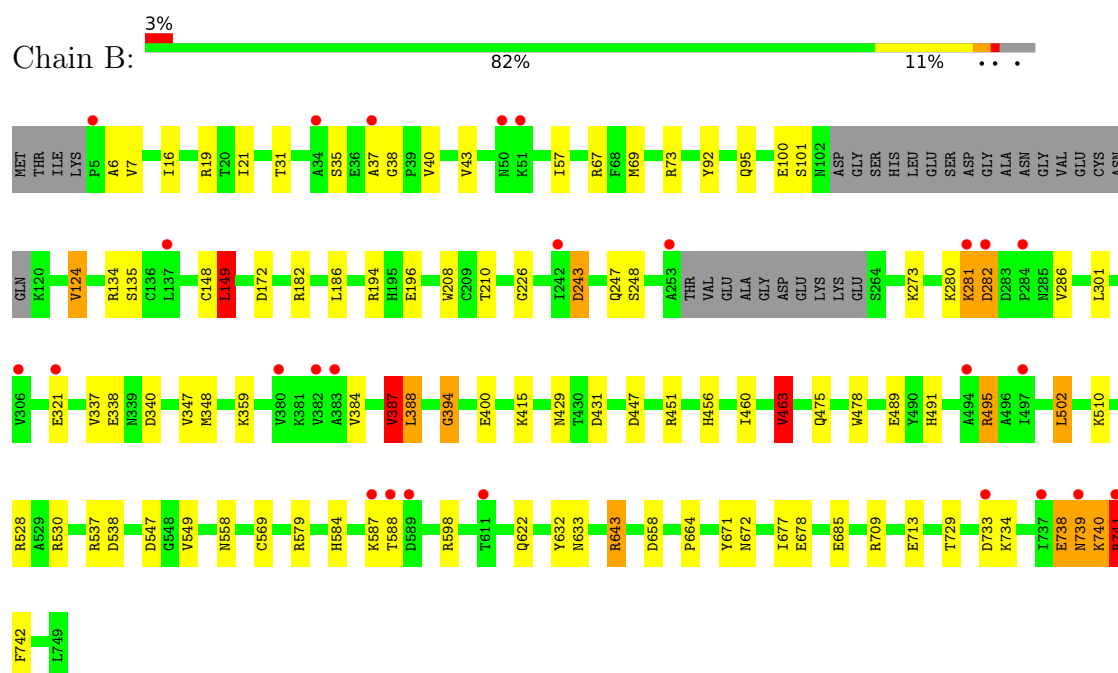
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	216	Total 216	O 216	0	0

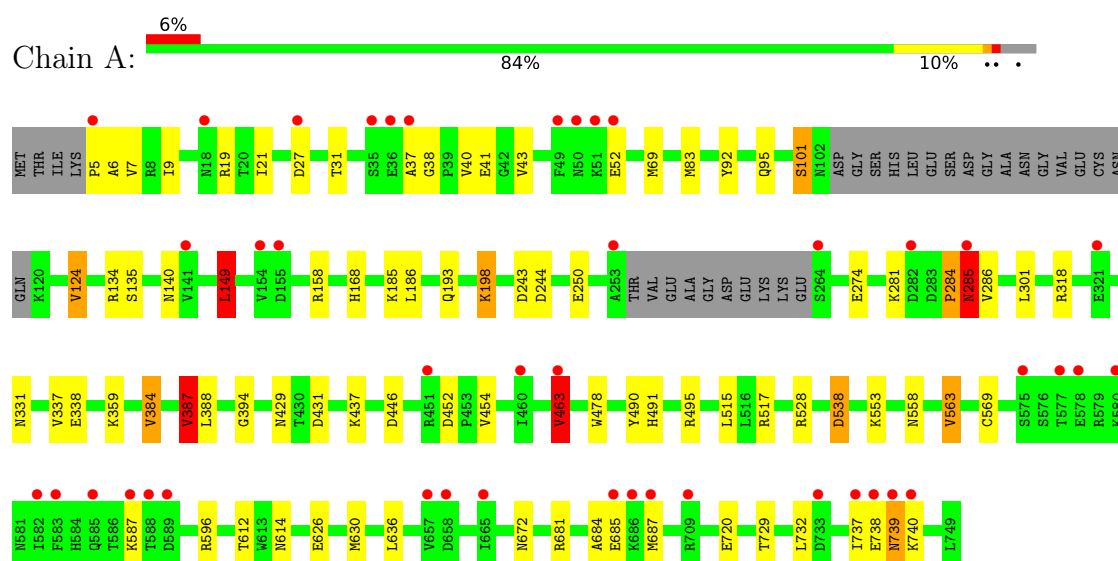
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Probable galactinol–sucrose galactosyltransferase 6



- Molecule 1: Probable galactinol–sucrose galactosyltransferase 6

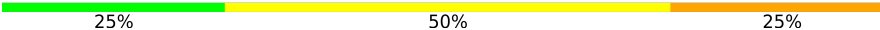


- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-idopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-psicofuranose

Chain C:  25% 50% 25%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-idopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-psicofuranose

Chain D:  25% 50% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.59Å 103.75Å 182.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.00) 99.8 (29.84-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.167 , 0.206 0.176 , 0.211	Depositor DCC
R_{free} test set	6172 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11874	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TTV, GLA, GLC, ZCD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	2/5754 (0.0%)	0.99	20/7793 (0.3%)
1	B	0.96	4/5754 (0.1%)	1.10	39/7793 (0.5%)
All	All	0.94	6/11508 (0.1%)	1.04	59/15586 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ASN	C-N	-17.88	0.93	1.34
1	A	284	PRO	C-N	-15.40	0.98	1.34
1	B	538	ASP	CB-CG	-6.68	1.37	1.51
1	B	196	GLU	CD-OE1	5.75	1.31	1.25
1	B	569	CYS	CB-SG	-5.30	1.73	1.81

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	ARG	NE-CZ-NH2	-16.89	111.85	120.30
1	B	530	ARG	NE-CZ-NH1	16.51	128.56	120.30
1	A	284	PRO	O-C-N	11.94	141.81	122.70
1	A	284	PRO	CA-C-N	-9.46	96.38	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ASN	O-C-N	-8.70	108.78	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	394	GLY	Peptide
1	A	684	ALA	Peptide
1	B	394	GLY	Peptide
1	B	740	LYS	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5620	0	5537	37	0
1	B	5620	0	5539	43	0
2	C	45	0	19	3	0
2	D	45	0	19	0	0
3	A	216	0	0	4	0
3	B	328	0	0	9	0
All	All	11874	0	11114	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 82 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:TTV:C5	2:C:1:TTV:O5	1.63	1.17
1:B:95:GLN:HE21	1:B:134:ARG:HH21	1.21	0.88
1:B:210:THR:OG1	3:B:801:HOH:O	1.91	0.88
1:B:738:GLU:HB3	1:B:739:ASN:HB2	1.57	0.85
1:A:284:PRO:O	1:A:285:ASN:CB	2.28	0.82

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	712/749 (95%)	673 (94%)	33 (5%)	6 (1%)	19	13
1	B	712/749 (95%)	680 (96%)	29 (4%)	3 (0%)	34	30
All	All	1424/1498 (95%)	1353 (95%)	62 (4%)	9 (1%)	25	19

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	282	ASP
1	B	741	ARG
1	A	6	ALA
1	A	285	ASN
1	A	685	GLU

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	614/640 (96%)	582 (95%)	32 (5%)	23	19
1	B	614/640 (96%)	581 (95%)	33 (5%)	22	18
All	All	1228/1280 (96%)	1163 (95%)	65 (5%)	22	18

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	563	VAL

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Mol	Chain	Res	Type
1	A	596	ARG
1	B	622	GLN
1	B	588	THR
1	A	612	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	456	HIS
1	A	739	ASN
1	A	558	ASN
1	A	385	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	TTV	C	1	2	11,12,12	5.18	5 (45%)	10,18,18	1.16	1 (10%)
2	GLC	C	2	2	11,11,12	2.12	3 (27%)	15,15,17	2.02	4 (26%)
2	ZCD	C	3	2	11,11,12	1.72	3 (27%)	15,15,17	2.09	5 (33%)
2	GLA	C	4	2	11,11,12	1.94	2 (18%)	15,15,17	0.92	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TTV	D	1	2	11,12,12	5.00	5 (45%)	10,18,18	1.10	1 (10%)
2	GLC	D	2	2	11,11,12	1.80	2 (18%)	15,15,17	2.78	5 (33%)
2	ZCD	D	3	2	11,11,12	1.23	1 (9%)	15,15,17	1.41	2 (13%)
2	GLA	D	4	2	11,11,12	0.96	0	15,15,17	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TTV	C	1	2	1/1/4/4	3/5/24/24	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1
2	ZCD	C	3	2	2/2/4/5	1/2/19/22	0/1/1/1
2	GLA	C	4	2	-	0/2/19/22	0/1/1/1
2	TTV	D	1	2	1/1/4/4	3/5/24/24	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	ZCD	D	3	2	2/2/4/5	1/2/19/22	0/1/1/1
2	GLA	D	4	2	-	0/2/19/22	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	TTV	C4-C5	-9.73	1.28	1.53
2	D	1	TTV	C4-C5	-9.41	1.28	1.53
2	C	1	TTV	O5-C5	9.01	1.63	1.43
2	D	1	TTV	O5-C5	8.84	1.63	1.43
2	C	1	TTV	O5-C2	8.58	1.56	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	O3-C3-C4	-6.20	96.02	110.35
2	D	2	GLC	O3-C3-C2	5.84	121.18	109.99
2	D	2	GLC	O2-C2-C3	4.16	118.47	110.14
2	C	3	ZCD	C1-C2-C3	4.08	114.68	109.67
2	C	2	GLC	O5-C5-C4	4.07	120.72	110.83

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	TTV	C3
2	C	3	ZCD	C2
2	C	3	ZCD	C3
2	D	1	TTV	C3
2	D	3	ZCD	C2

5 of 9 torsion outliers are listed below:

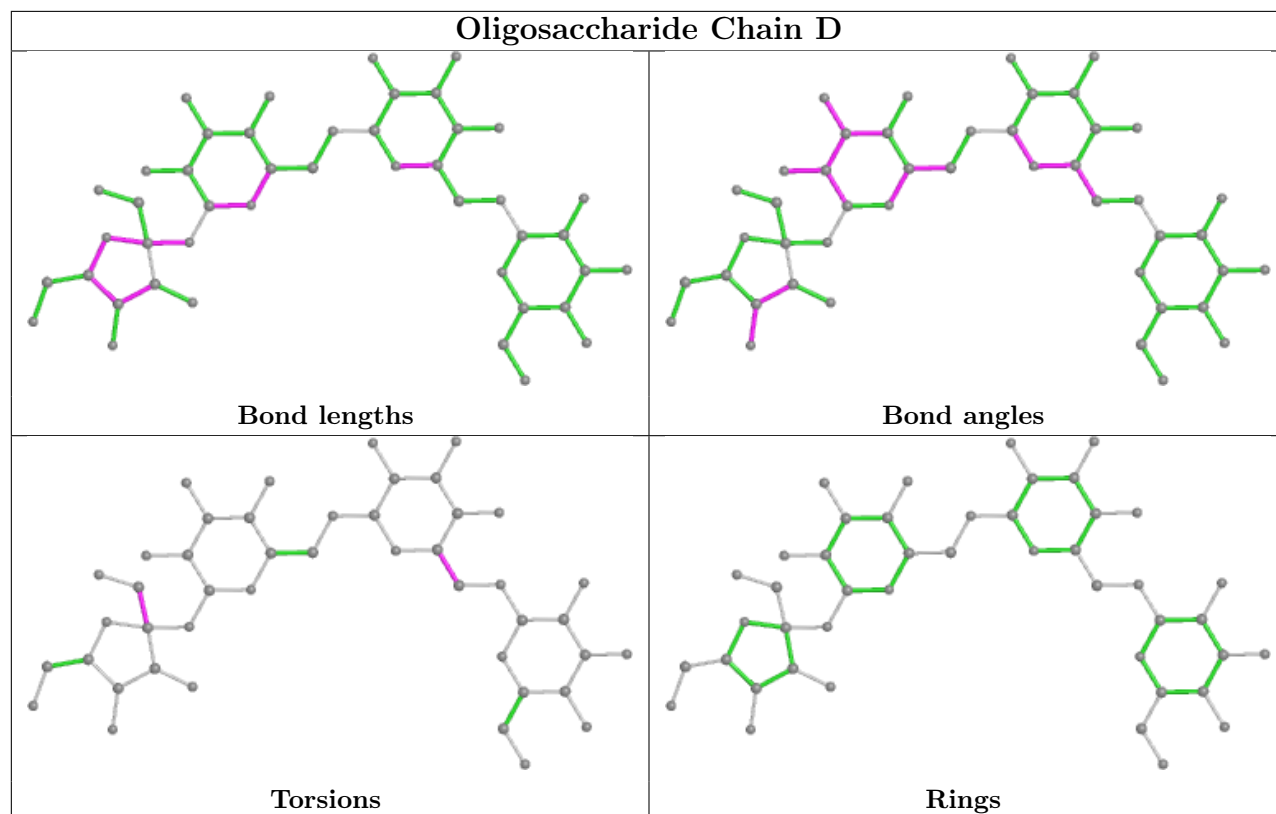
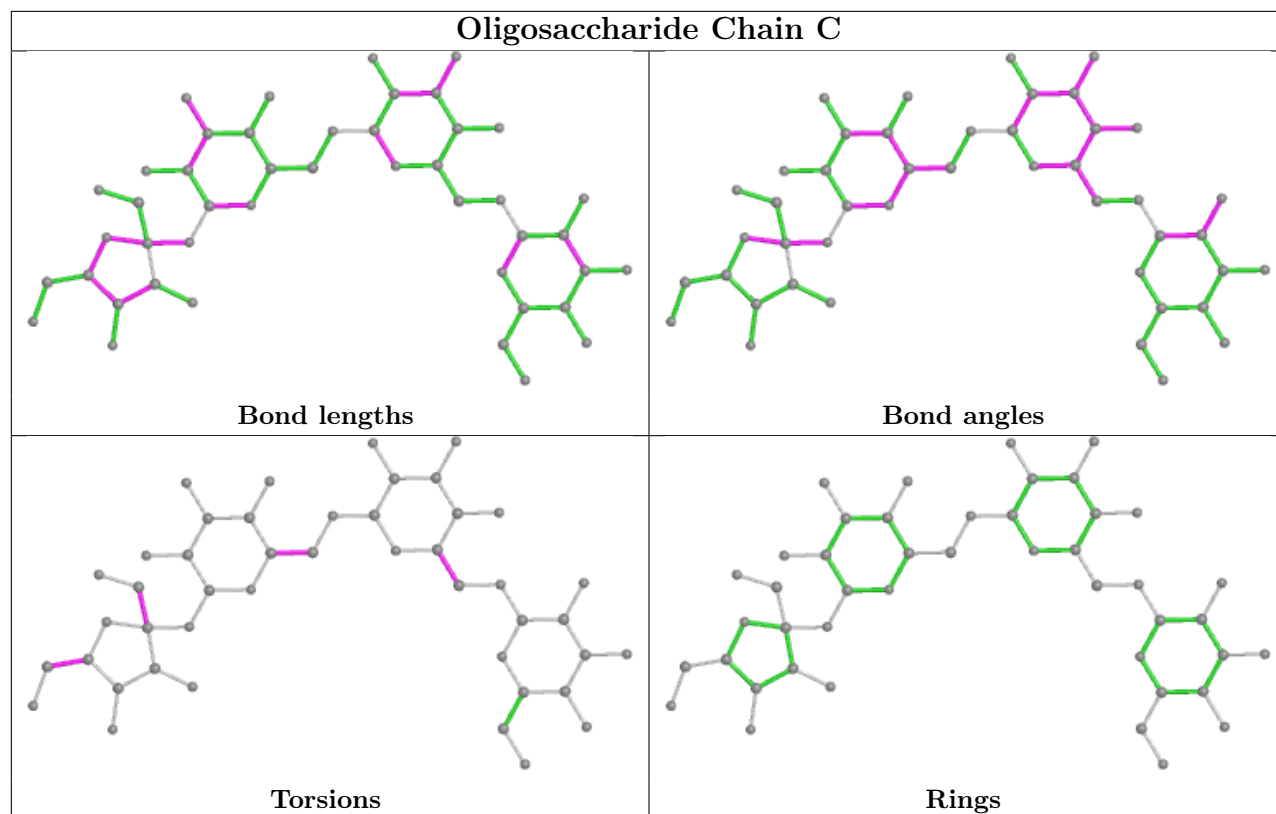
Mol	Chain	Res	Type	Atoms
2	D	1	TTV	O1-C1-C2-O2
2	C	1	TTV	O5-C5-C6-O6
2	D	1	TTV	O1-C1-C2-O5
2	C	2	GLC	C4-C5-C6-O6
2	C	1	TTV	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	ZCD	1	0
2	C	1	TTV	1	0
2	C	2	GLC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	284:PRO	C	285:ASN	N	0.98
1	A	285:ASN	C	286:VAL	N	0.92

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	718/749 (95%)	0.12	43 (5%) 21 20	27, 42, 74, 122	0
1	B	718/749 (95%)	-0.07	26 (3%) 42 42	25, 34, 60, 99	0
All	All	1436/1498 (95%)	0.03	69 (4%) 30 29	25, 39, 69, 122	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ALA	10.0
1	A	285	ASN	5.4
1	A	658	ASP	5.4
1	A	50	ASN	4.7
1	A	588	THR	4.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

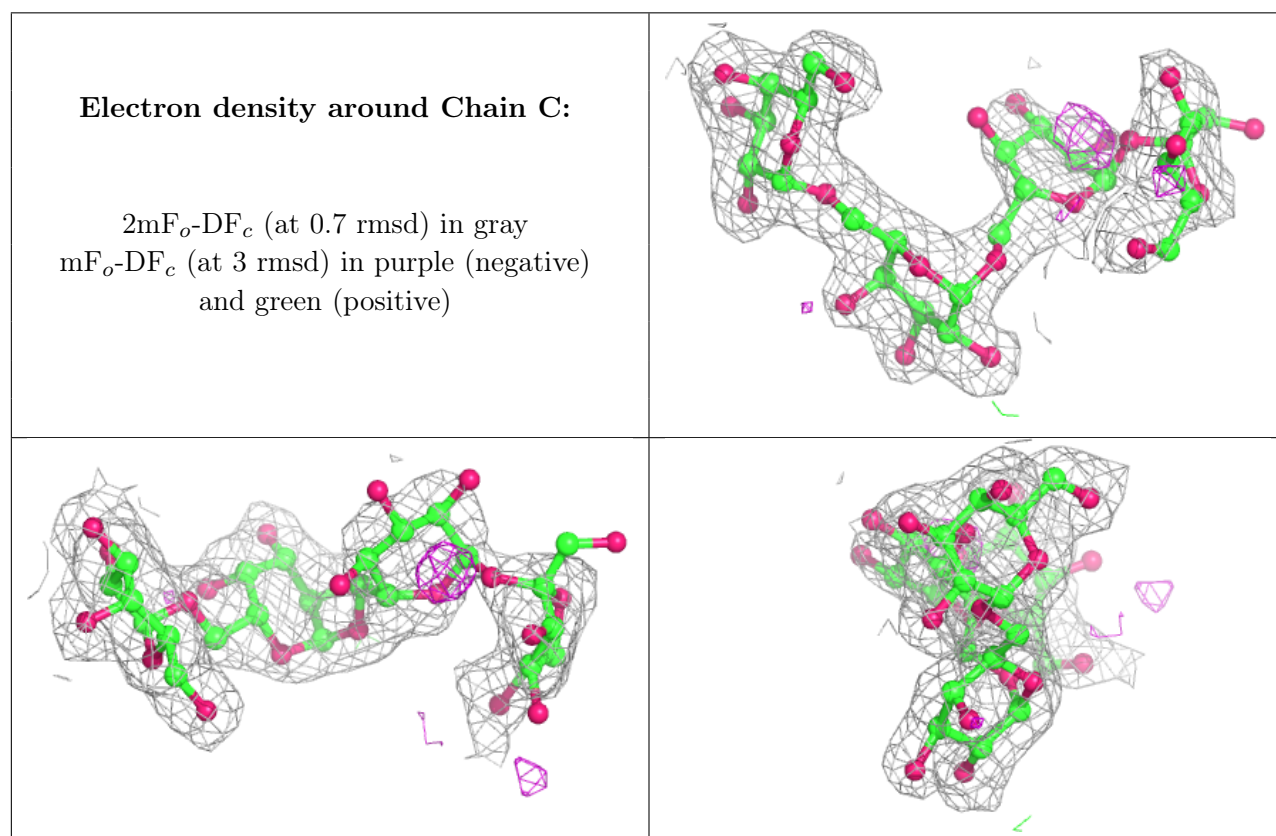
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TTV	C	1	12/12	0.78	0.47	76,94,107,113	0
2	GLC	C	2	11/12	0.84	0.38	59,81,91,94	0
2	GLC	D	2	11/12	0.88	0.25	40,52,60,63	0
2	TTV	D	1	12/12	0.90	0.39	56,70,72,83	0
2	ZCD	D	3	11/12	0.94	0.09	25,31,35,37	0

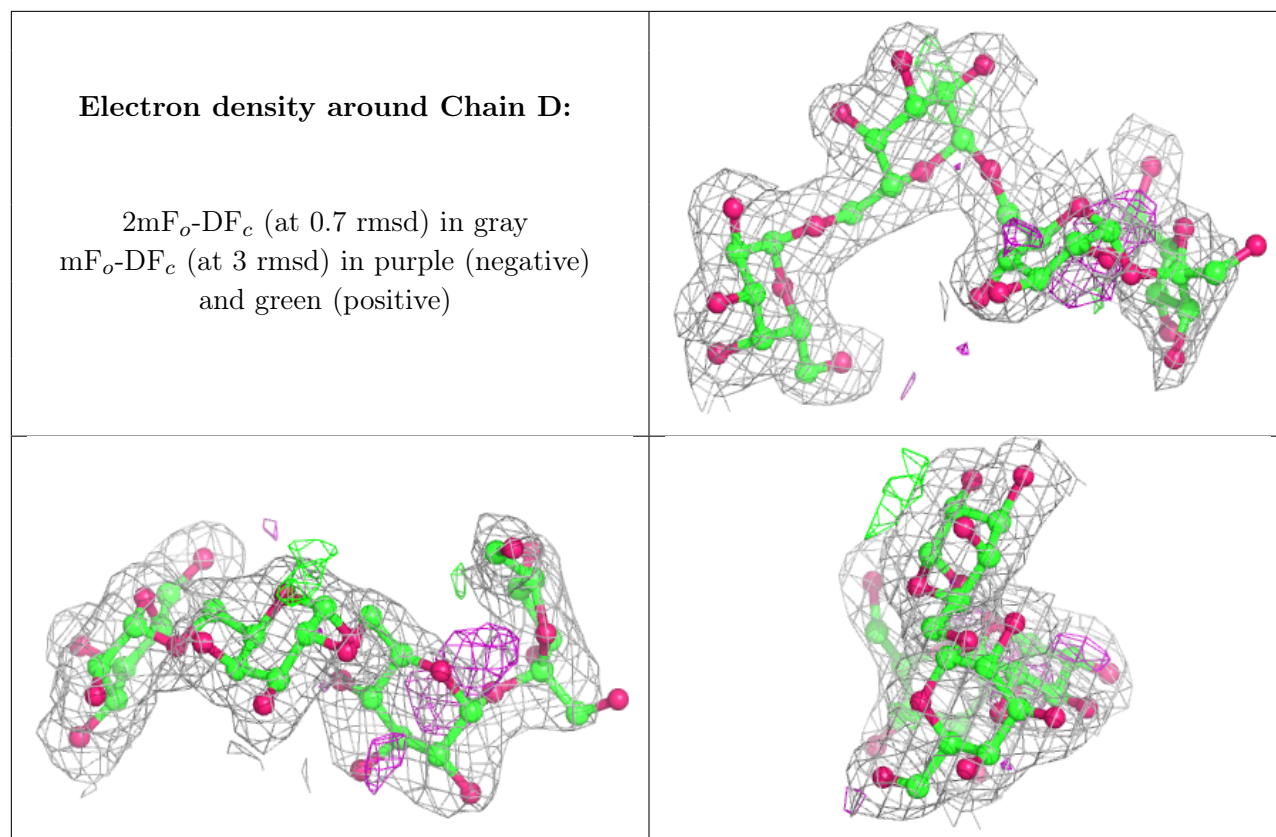
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZCD	C	3	11/12	0.95	0.10	33,46,49,54	0
2	GLA	C	4	11/12	0.98	0.09	30,32,34,36	0
2	GLA	D	4	11/12	0.98	0.13	24,26,29,30	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.